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Shear viscosity of polymer nanocomposites from NEMD simulations JAGANNATHAN T. KALATHI, SANAT K. KUMAR, Columbia University, GARY S. GREST, Sandia National Laboratories — Polymer nanocomposites (PNC) are preferred for a variety of applications since they offer excellent thermal, electrical, and mechanical properties. The viscosity of PNC is primarily a strong function of filler size. For micron-sized fillers, the shear viscosity increases with filler volume fraction following the well-known Einstein relationship. However as the particle size approaches the nanoscale, the viscosity is found to either increase or decrease depending on the strength of interactions between the particle and polymer. In this study, the shear viscosity of an entangled polymer melt of N=400 beads of diameter σ with and without fillers is estimated using NEMD simulations. The diameter of the nanoparticles (1-10σ) and volume fraction (0.05-0.3) are varied for shear rate from 10^{-2} to $10^{-6}\tau^{-1}$. The viscosity of PNC decreases when compared to pure melt for nanoparticles of size 1σ and recovers to the value of a pure melt when the size approaches 10σ, provided all the interactions are neutral. It thus appears that the increase in viscosity embodied in the Einstein relationship only manifests itself for large nanoparticle size >10σ.

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